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Invariant Imbedding, Iterative Linearization, and Multistage Countercurrent Processes. VII. Distillation Column at Minimum Reflux and Nonlinear Boundary Value Problems*

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The concept of treating multicomponent distillation problems as nonlinear boundary value problems in difference equations is used to solve columns at minimum reflux. Various computational algorithms are formulated based on the choice of different unknown variables and different boundary conditions. To show the quadratic convergence some typical algorithms are illustrated by numerical examples. It is shown that using very rough initial approximations or starting values, four to five digit accuracy is obtained in five to seven iterations.

1. INTRODUCTION

The basic concept of treating multicomponent distillation columns as nonlinear boundary value problems in difference equations can be extended easily to a distillation column at minimum reflux. By definition, a column at minimum reflux has an infinite number of stages at both the rectifying and stripping pinches. In other words, the compositions remain constant at the two pinch sections. Thus, each pinch section can be considered as one stage and can be represented by the pinch equation.

Based on the ideas developed in this series of papers [1, 2], various computational algorithms can again be developed for the nonlinear boundary value problem representing a column at minimum reflux. Some of the typical

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algorithms are developed and illustrated in this paper. The first aspect explored concerns the various boundary conditions which can be formulated for a column at minimum reflux. This is due to the fact that, in addition to the regular boundary conditions, the two pinch section conditions form ideal boundary conditions in formulating the boundary value problem. Another aspect concerns the choice of unknown variables. In addition to the regular concentration variables, total liquid and vapor phases flow rates, and temperature can also be used as the unknown variables.

2. Distillation Column at Minimum Reflux

The equations representing a multicomponent column with a total condenser were derived by Noh and Lee [1] using composition as the unknown variables. The equations for a column with a partial condenser can be obtained in a similar manner. These equations are

$$\Phi_i(0) = V(1)\, k_i(1)\, x_i(1) - L(0)\, x_i(0) - Dk_i(0)\, x_i(0) = 0, \quad i = 1,2,...,m, \quad (1)$$

$$\begin{aligned}\Phi(n) = {} & [k_i(n+1)\, x_i(n+1) - k_i(0)\, x_i(0)] \sum_{j=1}^{m} x_j(n)\, h_j(n) \\ & + [k_i(0)\, x_i(0) - x_i(n)] \sum_{j=1}^{m} k_j(n+1)\, x_j(n+1)\, H_j(n+1) \\ & + [x_i(n) - k_i(n+1)\, x_i(n+1)]u = 0, \qquad i = 1, 2,..., m. \end{aligned} \quad (2a)$$

The n is Eq. (2a) is

$$n = 1, 2,..., f-1, \quad (2b)$$

$$\begin{aligned}\Phi_i(n) = {} & [k_i(n+1)x_i(n+1) - (F/B)x_{if} + (D/B)k_i(0)x_i(0)] \sum_{j=1}^{m} x_j(n)h_j(n) \\ & + [(F/B)x_{if} - (D/B)k_i(0)x_i(0) - x_i(n)] \sum_{j=1}^{m} x_j(n+1)k_j(n+1) \\ & \times H_j(n+1) + [x_i(n) - k_i(n+1)x_i(n+1)]w = 0, \; i = 1, 2,..., m. \end{aligned} \quad (3a)$$

The n in Eq. (3a) is

$$n = f, \quad f+1,..., \quad N, \quad (3b)$$

with

$$u = (Q_c/D) + \sum_{j=1}^{m} k_j(0)\, x_j(0)\, H_j(0), \quad (4)$$

$$w = (1/B)\left[F \sum_{j=1}^{m} x_{jf} h_{jf} - Q_c - D \sum_{j=1}^{m} k_j(0)\, x_j(0)\, H_j(0)\right]. \quad (5)$$

For a partial condenser, the condenser duty Q_c can be represented by

$$Q_c = V(1) \sum_{j=1}^{m} x_j(1)\, k_j(1)\, H_j(1) - D \sum_{j=1}^{m} x_j(0)\, k_j(0)\, H_j(0) - L(0) \sum_{j=1}^{m} x_j(0)\, h_j(0), \tag{6}$$

where $x_i(n)$ represents the mole fraction of component i in the liquid stream leaving stage n. There are total m components in the system. The plates are numbered consecutively down from the top of the column. The condenser is the zeroth stage and the reboiler stage is $(N + 1)$. The symbols k, h, and H represent the equilibrium ratio, liquid enthalpy, and vapor enthalpy, respectively. The rates F, B, and D represent the total molal rates of the feed, the bottom stream, and the distillate stream, respectively. The feed stage is numbered f and the subscript f represents the feed stream conditions. The total vapor molal flow rate leaving stage one is represented by $V(1)$, and $L(0)$ represents the total liquid molal flow rate leaving stage zero.

Equation (1) represents the condenser. Equations (2) and (3) represent the recitfying and stripping sections, respectively. Equations (1)–(3) represent m nonlinear first order difference equations over the entire column including the condenser and the reboiler. The m unknowns are $x_i(n)$, $i = 1, 2,..., m$. The m boundary conditions for Eqs. (1)–(3) are

$$Fx_{if} = Bx_i(N + 1) + Dk_i(0)\, x_i(0), \qquad i = 1, 2,..., m, \tag{7}$$

where a partial condenser has been assumed in obtaining this equation. Equations (1)–(3) and (7) represent a nonlinear boundary value problem in difference equations. This problem was solved by quasilinearization in an earlier paper [1].

For a column at minimum reflux, there are an infinite number of plates in both the rectifying and stripping sections. In other words, there exist rectifying and stripping pinch regions within which there is no change in composition from plate to plate. Thus,

$$x_i(r + 1) = x_i(r), \qquad i = 1, 2,..., m, \tag{8}$$

where r represents the plate number at the rectifying pinch region. Equation (2a) at this pinch region becomes

$$\Phi_i(r - 1) = [k_i(r)\, x_i(r) - k_i(0)\, x_i(0)] \sum_{j=1}^{m} x_j(r)\, h_j(r) + [k_i(0)\, x_i(0) - x_i(r)] \sum_{j=1}^{m} k_j(r)\, x_j(r)\, H_j(r) + [x_i(r) - k_i(r)\, x_i(r)]u = 0, \qquad i = 1, 2,..., m. \tag{9}$$

At the stripping pinch region, we have

$$x_i(s+1) = x_i(s), \qquad i = 1, 2,..., m, \tag{10}$$

where s represents the plate number at the stripping pinch region. Using Eq. (10), Eq. (3a) for the stripping pinch region becomes

$$\Phi_i(s) = [k_i(s)\, x_i(s) - (F/B)\, x_{if} + (D/B)\, k_i(0)\, x_i(0)] \sum_{j=1}^{m} x_j(s)\, h_j(s)$$

$$+ [(F/B)\, x_{if} - (D/B)\, k_i(0)\, x_i(0) - x_i(s)] \sum_{j=1}^{m} x_j(s)\, k_j(s)\, H_j(s)$$

$$+ [x_i(s) - k_i(s)\, x_i(s)]w = 0, \qquad i = 1, 2,..., m. \tag{11}$$

Because of the presence of the pinch region, Eqs. (2a) and (3a) no longer represent the entire rectifying and stripping sections. Thus, Eqs. (2b) and (3b) become

$$n = r, \qquad r+1,..., f-1 \tag{2c}$$

$$n = f, \qquad f+1,..., s. \tag{3c}$$

3. A Nonlinear Boundary Value Problem in First Order Difference Equations

Equations (1)–(11) represent the desired equations. Notice that Eqs. (1), (9), (2a), and (3a) represent the zeroth stage, the rectifying pinch, the rectifying section below the pinch, and the stripping section above the pinch, respectively. Since the rth stage can be calculated once the x's, for the zeroth and first stages are known, Eq. (9) is essentially a first order difference equation with r equal to three. Thus, Eqs. (1), (2a), (3a), and (9) represent m first order difference equations over the column including the condenser and the stripping pinch section. The m unknowns are $x_i(n)$, $i = 1, 2,..., m$. Either Eq. (10) or Eq. (11) can be used as the m boundary conditions. Since both the initial stage $x_i(0)$ and the final stage $x_i(s)$ are present in Eq. (11), this equation forms a set of nonlinear mixed boundary conditions. Apparently, this set of nonlinear mixed boundary conditions. Apparently, this set of nonlinear conditions cannot be solved very easily. Thus, Eq. (10) will be used as the boundary conditions in the following calculations.

For the above multicomponent distillation column at minimum reflux, several different types of specifications may be made. We have assumed the following specifications: the composition, thermal condition and total molal rate of feed, the column pressure, the type of condenser, and an infinity of

plates in both the rectifying and stripping sections. In addition, two of three flow rates D, $V(1)$, and $L(0)$ are specified. With these specifications, we wish to obtain the product distribution. Notice that with the specification of any two of the three flow rates D, $V(1)$, and $L(0)$, the third flow rate can be calculated by using the total material balance around the condenser. The enthalpies h and H and the equilibrium ratio k are not unknowns. They are functions of the temperature T which, in turn, is a function of composition through the bubble point equation

$$\sum_{j=1}^{m} k_j(n)\, x_j(n) - 1 = 0. \tag{12}$$

Thus, k, h, and H are implicit functions of x.

Equations (1), (2a), (2c), (3a), (3c), (9), and (10) represent a nonlinear boundary value problem in first order difference equations. This sytem of equations can be solved by quasilinearization [3]. Equations (1), (2a), (2c), (3a), (3c), and (9) can be represented symbolically:

$$\Phi(n) = \Phi(x(0), x(1), x(r), x(n), x(n+1)) = 0, \qquad n = 0, 1, 2, \ldots, s, \tag{13}$$

where Φ and x represent m-dimensional vectors. The above equation can be linearized as [3]

$$\begin{aligned}\Phi(n) &+ J_{x(0)}[x_{k+1}(0) - x_k(0)] + J_{x(1)}[x_{k+1}(1) - x_k(1)] \\ &+ J_{x(r)}[x_{k+1}(r) - x_k(r)] + J_{x(n)}[x_{k+1}(n) - x_k(n)] \\ &+ J_{x(n+1)}[x_{k+1}(n+1) - x_k(n+1)] = 0.\end{aligned} \tag{14}$$

Where the subscript k indicates variables obtained in the previous kth iteration and variables with subscript $k+1$ are unknown current $(k+1)$st iteration variables. All the variables in the Jacobian matrix J are kth iteration variables. The elements of the $m \times m$ Jacobian matrix J_x can be obtained by partial differentiation of Eq. (13) with respect to x. For example, the elements for $J_{x(m)}$ for the rectifying section below the rectifying pinch are

$$\begin{aligned}\partial\Phi_i(n)/\partial x_l(n) = &\left[U - \sum_{j=1}^{m} k_j(n+1)\, x_j(n+1)\, H_j(n+1)\right]\delta_{il} \\ &+ [k_i(n+1)\, x_i(n+1) - k_i(0)\, x_i(0)] \\ &\times \left[h_l(n) + \sum_{j=1}^{m} x_j(n)\left(\partial h_j(n)\Big/\partial x_l(n)\right)\right], \\ &\qquad i, l = 1, 2, \ldots, m, \quad n = r, r+1, \ldots, f-1,\end{aligned} \tag{15}$$

where

$$\begin{aligned} \delta &= 1, \qquad i = l, \\ il &= 0, \qquad i \neq l. \end{aligned} \tag{16}$$

Since h is a function of T, we have

$$\partial h_j(n)/\partial x_l(n) = (dh_j(n)/dT(n))(\partial T(n)/\partial x_l(n)).$$

Using Eq. (11), we have

$$\partial T(n)/\partial x_l(n) = -k_l(n)\Big/\sum_{j=1}^{m} x_j(n)(dk_j(n)/dT). \tag{17}$$

The elements for other Jacobians and for other sections of the column can be obtained in a similar manner.

Since k, h, and H are functions of x's through T, implicit differentiation must be used to linearize the equations involving these parameters. As can be seen from Eq. (17), the resulting equations from these implicit differentiations can be very complicated. In order to retain the quadratic convergence property of quasilinearization, all three parameters, k, h, and H, should be considered in the linearization. However, practical experience indicates [1] that if all three parameters are considered in linearization, the resulting linearized expression is so complicated that unreasonably large or small values are obtained for the particular and homogenous solutions. On the other hand, if none of the three parameters are considered in the linearization, the convergence rate becomes too slow. In this work, a compromise is used and only k is not considered in the linearization. Both h and H are linearized by the use of implicit differentiation.

4. Numerical Example

To illustrate the approach and also to compare with existing techniques, a problem solved by Holland [3] is solved. The problem has five components. The numerical values used are

$$\begin{gathered} F = 100, \qquad V(1) = 55, \qquad D = 40, \qquad m = 5, \\ x_{if} = 0.2, \qquad i = 1, 2, \ldots, 5. \end{gathered} \tag{18}$$

A partial condenser is used and the column pressure is 400 psia. Boiling point liquid is used as the feed. The values of k, h, and H have been correlated as functions of temperature for the various components by Holland [3]. The subscript i for $i = 1, 2, \ldots, 5$ denotes C_3H_8, $i - C_4$, $n - C_4$, $i - C_5$, and $n - C_5$, respectively.

Equations (14) and (10) form a linear boundary value problem. The general solution of the linear difference Eq. (14) is

$$x_{i,k+1}(n) = x_{ip,k+1}(n) + \sum_{j=1}^{m} a_j x_{ihj,k+1}(n), \qquad i = 1, 2,..., m, \quad n = 1, 2,..., N+1, \tag{19}$$

where the subscripts p and h indicate particular and homogeneous solutions. Substituting Eq. (19) into the boundary equation, Eq. (10), a system of linear algebraic equations with the integration constants a's as the only unknowns, are obtained. Once the values for the a's are obtained, the general solution for the (kth)st iteration can be obtained by using Eq. (19). This iterative process can be continued until the desired accuracy is obtained.

To start the first iteration, constant composition profiles are used as the initial approximation for the x's. In other words, the following constant initial approximations or starting values are used.

$$x_{1,k}(n) = 0.25, \quad x_{2,k=0}(n) = 0.25, \quad x_{3,k=0}(n) = 0.20, \quad x_{4,k=0}(n) = 0.15, \quad x_{5,k=0}(n) = 0.15, \quad \text{for all } n, \quad 0 \leqslant n \leqslant N+1. \tag{20}$$

Since the temperature T appears implicitly in all the equations where h, H, or k is present, the values of T are obtained after each quasilinearization iteration by solving Eq. (12). Newton's iteration method is used to solve Eq. (12).

For computational purposes, the number of stages used between the rectifying pinch and the stripping pinch must be considered carefully. In this work, seven stages were assumed between the two pinches. Three stages were assumed for the rectifying section, and three stages were assumed for the stripping section. In order to make sure that seven stages are satisfactory, the problem was also solved with nine stages. The same results were obtained with both seven and nine stages.

The initial conditions used are listed in Table I. The convergence rates of the liquid phase overhead composition and temperature are listed in Table II. Notice that in spite of the very approximate initial approximation, only five iterations are needed to obtain a four digits accuracy for the overhead concentration. A five digit accuracy in the overhead and pinch temperatures is obtained in only three and two iterations, respectively. This problem was solved by Holland. With a much better initial approximation for temperature, five to ten trials were needed to obtain a four or five digit accuracy [3]. Once the overhead composition is obtained, the bottom composition can be obtained by using Eq. (7).

TABLE I

Initial Conditions Used for Obtaining Particular and Homogeneous Solutions

Variable	Particular solution	Homogeneous solution				
		1	2	3	4	5
$x_1(0)$	0.2	0.2	0.05	0.2	0.2	0.2
$x_2(0)$	0.2	0.2	0.35	0.05	0.2	0.2
$x_3(0)$	0.2	0.2	0.2	0.35	0.05	0.2
$x_4(0)$	0.2	0.2	0.2	0.2	0.35	0.05
$x_5(0)$	0.2	0.2	0.2	0.2	0.2	0.35

TABLE II

Convergence Rates of Overhead Concentrations

Iteration	$x_1(0)$	$x_2(0)$	$x_3(0)$	$x_4(0)$	$x_5(0)$	$T(0)$	$T(r)$
0	0.25	0.25	0.20	0.15	0.15	712.22	712.22
1	0.2371	0.2179	0.1924	0.1429	0.1245	713.91	722.93
2	0.2439	0.2201	0.2049	0.1536	0.1310	713.48	726.98
3	0.2492	0.2265	0.2133	0.1642	0.1419	713.35	727.34
4	0.2496	0.2273	0.2142	0.1654	0.1432	713.32	727.34
5	0.2498	0.2274	0.2142	0.1654	0.1432	713.32	727.34
20	0.2498	0.2274	0.2142	0.1654	0.1432	713.32	727.34

5. Alternate Formulation

Because the problem is treated as a boundary value problem, many different formulations are possible. For example, the problem could be solved by considering the equations representing the reboiler, the stripping pinch, the stripping section, and the rectifying section below the rectifying pinch, with Eq. (8) as the boundary condition.

For illustrative purposes, we shall consider another different approach. Instead of Eq. (3a) or (11), the following equation for the stripping section can be obtained.

$$\begin{aligned}\Phi_i(n) = {} & [x_i(n-1) - x_i(N+1)] \sum_{j=1}^{m} x_j(n)\, k_j(n)\, H_j(n) \\ & + [x_i(N+1) - k_i(n)\, x_i(n)] \sum_{j=1}^{m} x_j(n-1)\, h_j(n-1) \\ & + [x_i(n-1) - k_i(n)\, x_i(n)](-w) = 0, \qquad (21) \\ i = {} & 1, 2, \ldots, m, \qquad n = f+1, f+2, \ldots, N+1,\end{aligned}$$

where $(N + 1)$ represents the reboiler stage. The above equation was obtained by considering material and enthalpy balances around the reboiler and by eliminating the vapor concentration and flow rates variables. At the stripping pinch section, Eq. (21) becomes

$$\Phi_i(s) = [x_i(s) - x_i(N+1)] \sum_{j=1}^{m} x_j(s)\, k_j(s)\, H_j(s) + [x_i(N+1) - k_i(s)\, x_i(s)] \sum_{j=1}^{m} x_j(s)\, h_j(s) + [x_i(s) - k_i(s)\, x_i(s)][-w] = 0, \qquad i = 1, 2, \ldots, m. \tag{22}$$

For the stripping section above the pinch, we have

$$n = f, f+1, \ldots, (s-1). \tag{3d}$$

If the concentration for the stripping pinch $x_i(s)$ is known, Eq. (22) can be used to calculate the bottom concentration $x_i(N + 1)$. Thus, Eqs. (1), (9), (2a), 2(c), (3a), (3d), and (22) form a system of m nonlinear first order difference equations representing the entire column including the condenser and the reboiler. Notice that Eqs. (9) and (22) are first order difference equations since in practice single stage numbers are assigned to each of the pinch sections. The m boundary conditions for this nonlinear system are represented by Eq. (7). If we consider each of the pinch sections as one stage, this system of nonlinear boundary value problems is very similar to that solved in [1]. Quasilinearization can again be used. Equations (1), (2a), (2c), (3a), (3d), (9), and (22) can be represented symbolically as

$$\Phi(n) = \Phi(x(0), x(1), x(r), x(n), x(n+1), x(s), x(N+1)) = 0, \tag{23}$$

where $n = 0, 1, 2, \ldots, N$ with $r = 2$ and $s = N$ in actual computations. The vectors Φ and x are m-dimensional vectors. Equation (23) can be linearized in the same way as that used to linearize Eq. (13) except that $x(s)$ and $x(N + 1)$ must also be considered in the linearization. The Jacobian matrix in the linearized equation can also be obtained in a similar way. Again, k was not considered in the linearization.

Using the numerical values listed in Eq. (18), and with the same assumed number of stages between the two pinch sections, this problem was solved. The same assumed initial approximations listed in Eq. (20) and the same assumed initial conditions listed in Table I are used. The convergence rates of the overhead concentrations and temperature, and the pinch section temperature are listed in Table III. It should be mentioned that because Eq. (7) is used as the boundary condition, and because $k_i(0)$ is an implicit function of $x_i(0)$, the boundary condition is no longer linear. In this work, Eq. (7), was considered linear and the value of $k_i(0)$ was considered known. In actual computation, the previous iteration results for $k_i(0)$ are used in the

current iteration calculations in Eq. (7). This undoubtedly slows down the convergence rate. However, as can be seen from Table III, the convergence rate was only slowed down slightly. It is true that Eq. (7) could be treated as a nonlinear equation by considering $k_i(0)$ as a function of $x_i(0)$ and by using Newton's iteration method to solve this boundary condition. However, it is believed that this nonlinear approach would require more computation time than the results obtained in Table III, although fewer iterations may be resulted.

TABLE III

Convergence Rates of the Alternate Formulation

Iteration	$x_1(0)$	$x_2(0)$	$x_3(0)$	$x_4(0)$	$x_5(0)$	$T(0)$	$T(r)$
0	0.25	0.25	0.20	0.15	0.15	712.22	712.22
1	0.2373	0.2196	0.1922	0.1405	0.1231	713.65	722.70
2	0.2385	0.2205	0.2077	0.1561	0.1330	714.52	727.79
3	0.2512	0.2263	0.2135	0.1655	0.1435	713.18	727.11
4	0.2500	0.2268	0.2136	0.1647	0.1424	713.25	727.29
5	0.2498	0.2274	0.2142	0.1653	0.1431	713.31	727.33
6	0.2498	0.2274	0.2142	0.1654	0.1432	713.32	727.34
10	0.2498	0.2274	0.2142	0.1654	0.1432	713.32	727.34

6. Liquid Flow Rate as One Unknown Variable—A System of Mixed Difference and Algebraic Equations

To illustrate another alternate formulation, the total liquid flow rate $L(n)$ will be considered as one of the m unknown variables. In other words, the m unknown variables are $x_i(n)$, $i = 1, 2,..., m - 1$, and $L(n)$. Notice that since the problem is considered as a nonlinear boundary value problem in difference equations, any of the parameters x, y, T, L, or V can be considered as the unknowns, where y is the vapor mole fraction.

Using the same nomenclature as before, the following m equations for the rectifying and stripping sections can be obtained.

$$\Phi_i(n) = [L(n) + D - \lambda F]\, x_i(n+1)\, k_i(n+1) - L(n)\, x_i(n) - D x_i(0)\, k_i(0) + \lambda F x_{if}, \qquad i = 1, 2,..., m-1, \tag{24a}$$

$$\Phi_m(n) = [L(n) + D - \lambda F] \sum_{j=1}^{m} x_j(n+1)\, k_j(n+1)\, H_j(n+1) - L(n) \sum_{j=1}^{m} x_j(n)\, h_j(n) - D \sum_{j=1}^{m} x_j(0)\, k_j(0)\, H_j(0) - Q_c + \lambda F \sum_{j=1}^{m} x_{jf} h_{jf}, \tag{24b}$$

with

$$n = 1, 2,..., N, \tag{24c}$$

$$\begin{aligned} \lambda &= 0, \qquad n = 1, 2,..., f-1, \\ &= 1, \qquad n = f, f+1,..., N. \end{aligned} \tag{25}$$

Since $x_m(n)$ is not considered as an unknown, this variable must be eliminated from Eq. (24b). This can be accomplished by using the equation

$$x_m(n) = 1 - \sum_{j=1}^{m-1} x_j(n). \tag{26}$$

Equation (24b) becomes

$$\begin{aligned} \Phi_m(n) = {} & [L(n) + D - \lambda F]\,\eta(n+1) - L(n)\,\zeta(n) \\ & - D\eta(0) - Q_c + \lambda F \sum_{j=1}^{m} x_{jf} h_{jf}\,, \end{aligned} \tag{24d}$$

where

$$\eta(n) = k_m(n)\,H_m(n) + \sum_{j=1}^{m-1} (x_j(n)[k_j(n)\,H_j(n) - k_m(n)\,H_m(n)]), \tag{27}$$

$$\zeta(n) = h_m(n) + \sum_{j=1}^{m-1} (x_j(n)[h_j(n) - h_m(n)]). \tag{28}$$

Equation (24a) represents the individual material balance after the total vapor rate $V(n+1)$ and the vapor mole fraction $y_i(n+1)$ have been eliminated from the equation, and Eq. (24b) represents the total enthalpy balance after similar manipulations.

Notice that in Eq. (24), $L(n)$ appears as an algebraic quantity, not as a first order difference quantity. Only $L(n)$ appears in these equations, while both $x_i(n)$ and $x_i(n+1)$ appear in the same equations. Thus, Eq. (24) is a system of first order difference equations for x_i and is only a system of algebraic equations for $L(n)$. Since $L(0)$ is a given quantity, only the following $(m-1)$ difference equations are needed for the condenser or zeroth stage.

$$\Phi_i(0) = V(1)\,k_i(1)\,x_i(1) - L(0)\,x_i(0) - Dk_i(0)\,x_i(0) = 0, \quad i = 1, 2,..., m-1. \tag{29}$$

For the rectifying pinch section, Eqs. (24a) and (24d) become

$$\begin{aligned} \Phi_i(r-1) = {} & [L(r) + D]\,x_i(r)\,k_i(r) - L(r)\,x_i(r) \\ & - Dx_i(0)\,k_i(0), \qquad i = 1, 2,..., m-1, \end{aligned} \tag{30a}$$

$$\Phi_m(r-1) = [L(r) + D]\,\eta(r) - L(r)\,\zeta(r) - D\xi(0) - Q_c\,. \tag{30b}$$

For a column at minimum reflux, Eq. (24c) becomes

$$n = r, \gamma + 1,..., s, \tag{24e}$$

with

$$\begin{aligned} \lambda &= 0, \quad n = r, r + 1,..., f - 1, \\ &= 1, \quad n = f, f + 1,..., s. \end{aligned} \tag{31}$$

Equations (29), (30), (24a), (24d), (24e), and (31) form a system of simultaneous nonlinear algebraic and difference equations representing the column above the stripping pinch including the condenser and the stripping pinch. Since there are only $(m - 1)$ first order difference variables $x_i(n)$, $i = 1, 2,..., m - 1$, $(m - 1)$ boundary conditions are needed. These $(m - 1)$ boundary conditions are

$$x_i(s) = x_i(s + 1), \qquad i = 1, 2,..., m - 1. \tag{32}$$

Equations (30), (24a), and (24d) can be represented symbolically as

$$\Phi(n) = \Phi(x(0), x(1), x(r), x(n), x(n + 1)) = 0, n = r - 1, r, r + 1,..., s, \tag{33}$$

where Φ and x represent m-dimensional vectors. The last elements in vectors (0), $x(1)$, and $x(n)$ are zero, and the last elements in the vectors $x(r)$ and $x(n + 1)$ are $L(r)$ and $L(n)$, respectively. For example, we have the vectors

$$x(r) = \begin{bmatrix} x_1(r) \\ x_2(r) \\ \vdots \\ x_{m-1}(r) \\ L(r) \end{bmatrix}, \qquad x(n + 1) = \begin{bmatrix} x_1(n + 1) \\ x_2(n + 1) \\ \vdots \\ x_{m-1}(n + 1) \\ L(n) \end{bmatrix}.$$

Equation (33) can be linearized in the same way as that used to linearize Eq. (13). The Jacobian matrices can again be obtained by partial differentiation. The parameter k_i is again not considered in the linearization. Thus, Eq. (29) is a linear equation. Notice that $L(0)$ and $V(1)$ are given quantities.

The system represented by Eqs. (29), (30), (24a), (24d), (24e), and (32) can again be solved by quasilinearization. The general solution for the linearized equation of Eqs. (29) and (33) can be represented by

$$\begin{aligned} x_{i,k+1}(n) &= x_{ip,k+1}(n) + \sum_{j=1}^{m-1} a_j x_{ihj,k+1}(n), \\ i &= 1, 2,..., m - 1, \quad n = 0, 1, 2,..., s + 1, \end{aligned} \tag{34}$$

$$L_{k+1}(n) = L_{p,k+1}(n), \qquad n = 1, 2,..., s. \tag{35}$$

Equation (35) is true only if the correct values for $x_i(0)$, $i = 1, 2,..., m - 1$, are used as the initial conditions to obtain the particular solutions. Since the correct values for $x_i(0)$ are the unknown we wish to obtain, some guessed values which may be fairly far removed from the correct values must be used for $x_{ip}(0)$. Thus, instead of Eq. (35), the following should be used for $L(n)$.

$$L_{k+1}(n) = L_{p,k+1}(n) + \sum_{j=1}^{m-1} a_j L_{hj,k+1}(n), \qquad n = 1, 2,..., s, \tag{36}$$

for the first few iterations. In actual computation, Eq. (36) was used during the first five iterations, and Eq. (35) was used after the fifth iteration. Thus, once the homogeneous and particular solutions are obtained, the $(m - 1)$ integration constants can be obtained by solving Eq. (34).

Using the numerical values listed in Eq. (18), this problem was solved by quasilinearization. To start the first iteration, the initial approximations listed in Eq. (20) for $x_{i,k=0}(n)$, $i = 1, 2, 3, 4$ are used. The initial approximation used for $L(n)$ is

$$L_{k=0}(n) = 15.0, \qquad n = r, r + 1,..., f - 1 \tag{37a}$$

$$L_{k=0}(n) = 115.0, \qquad n = f, \quad f + 1,..., s. \tag{37b}$$

Notice that the value of $L(0)$ is used as the initial approximation for the rectifying section, and $L(0) + F$ is used for the stripping section.

The values listed in Table I for the first four sets of homogeneous solutions are used as the initial conditions for the four sets of homogeneous solutions. For the particular solutions, the following initial conditions are used.

$$x_{ip,k+1}(0) = x_{ik}, \qquad i = 1, 2, 3, 4. \tag{38}$$

TABLE IV

Convergence Rates with L as an Unknown

Iteration	$x_1(0)$	$x_2(0)$	$x_3(0)$	$x_4(0)$	$L(1)$	$T(0)$	$T(r)$
0	0.25	0.25	0.20	0.15	15.0	712.22	712.22
1	0.2356	0.2032	0.1854	0.1221	17.1	721.34	727.53
2	0.2474	0.2187	0.2025	0.1442	17.6	715.75	727.33
3	0.2485	0.2244	0.2105	0.1594	15.3	714.22	727.34
4	0.2500	0.2265	0.2127	0.1621	15.2	713.52	727.34
5	0.2496	0.2271	0.2139	0.1651	14.7	713.41	727.34
6	0.2499	0.2273	0.2140	0.1649	14.8	713.32	727.34
7	0.2498	0.2274	0.2142	0.1654	14.7	713.32	727.34
20	0.2498	0.2274	0.2142	0.1654	14.7	713.32	727.34

In other words, the general solutions of the previous iterations are used as the initial conditions for the particular solutions of the current iteration. The convergence rate for this problem is listed in Table IV. Because of the requirement of using the exactly correct initial condition for particular solutions and the simultaneous solution of algebraic and difference equations. The convergence rate is not as fast as that listed in Table II. Seven iterations are needed to obtain a four digit accuracy for the overhead concentration.

7. Discussion

Since the problem is treated as a nonlinear boundary value problem in difference equations, many alternate formulations are possible. Because of space limitation, only some typical formulations are illustrated in this paper. For example, temperature can also be considered as one unknown variable. Another approach would be to calculate the column in two sections and use the boundary condition at the feed stage to match the results.

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